

Message

---

**From:** Mei Sun [Mei.Sun@uncc.edu]  
**Sent:** 9/22/2020 3:59:41 PM  
**To:** McCord, James [mccord.james@epa.gov]  
**CC:** Strynar, Mark [Strynar.Mark@epa.gov]; Yen-Ling Liu [yliu81@uncc.edu]  
**Subject:** Re: structure confirmation of nafion byproduct 4

Got it. Thank you.

Mei Sun

Assistant Professor  
Department of Civil and Environmental Engineering  
University of North Carolina at Charlotte  
Energy Production and Infrastructure Center 3163  
9201 University City Blvd | Charlotte, NC 28223  
Phone: 704-687-1723 | Fax: 704-687-0957  
Website: <https://coefs.uncc.edu/msun8/>

On Tue, Sep 22, 2020 at 11:51 AM McCord, James <mccord.james@epa.gov> wrote:

I don't think those isomers can be uniquely distinguished via MS/MS. We see multiple isomers for most of the Nafion byproducts so it is normally a combination. I would go with what NCDEQ/Chemours have settled on.

--

James McCord

---

**From:** Strynar, Mark  
**Sent:** Tuesday, September 22, 2020 11:22 AM  
**To:** [Mei.Sun@uncc.edu](mailto:Mei.Sun@uncc.edu); McCord, James <mccord.james@epa.gov>  
**Cc:** Yen-Ling Liu <yliu81@uncc.edu>  
**Subject:** RE: structure confirmation of nafion byproduct 4

Hi Mei,

Per the attached Excel file from Chemours to NCDEQ they draw the structure as the top one (row 9). However I am unsure if James saw both isomers in the work we presented in the ES&T paper you referenced in Figure 86 and in Table S2 both may be real. I will let him tell you for sure.

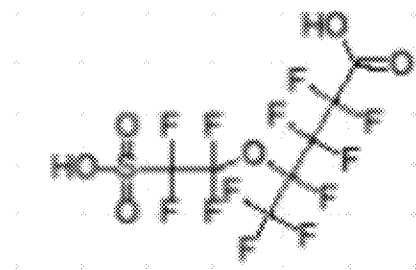
Mark

**From:** Mei Sun <Mei.Sun@uncc.edu>  
**Sent:** Tuesday, September 22, 2020 10:04 AM  
**To:** Strynar, Mark <Strynar.Mark@epa.gov>  
**Cc:** Yen-Ling Liu <yliu81@uncc.edu>  
**Subject:** structure confirmation of nafion byproduct 4

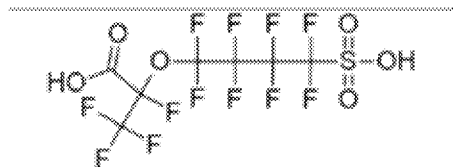
Hi Mark

I am working on PFAS paper and would like to confirm with you the chemical structure of NBP4. Based on the formula of C<sub>7</sub>H<sub>2</sub>F<sub>12</sub>O<sub>6</sub>S people use for Nafion byproduct 4, I found two isotherms in your paper (<https://pubs.acs.org/doi/10.1021/acs.est.8b06017>):

This one is from Figure 86 in the SI:



And this one is from line 22 of Table S2



When searching in the EPA dashboard with the CAS 852157-01-8 in Table S2, I found the second structure too. So could you please confirm which, if any, should be the right structure for NBP4? Thank you.

Mei Sun

Assistant Professor  
Department of Civil and Environmental Engineering  
University of North Carolina at Charlotte  
Energy Production and Infrastructure Center 3163  
9201 University City Blvd | Charlotte, NC 28223  
Phone: 704-687-1723 | Fax: 704-687-0957  
Website: <https://coefs.uncc.edu/msun8/>